Thermalization of Interacting Fermions and Delocalization in Fock space

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By means of exact diagonalization, we investigate the onset of 'eigenstate thermalization' and the crossover to ergodicity in a system of 1D fermions with increasing interaction. We show that the fluctuations in the expectation values of the momentum distribution from eigenstate to eigenstate decrease with increasing coupling strength and system size. It turns out that these fluctuations are proportional to the inverse participation ratio of eigenstates represented in the Fock basis. We demonstrate that eigenstate thermalization should set in even for vanishingly small perturbations in the thermodynamic limit.

Introduction. – Statistical physics relies on the assumption that the system under investigation is in thermal equilibrium. However, what are the precise conditions for an isolated system to relax to thermal equilibrium? This question has a long history including the ground breaking numerical experiments initiated by Fermi, Pasta and Ulam [1] on an anharmonic chain of classical oscillators, where thermalization was not observed as expected [2]. Nowadays, the investigation of thermalization in quantum many-body systems attracts a lot of theoretical attention, inspired by the new experimental possibilities in systems of cold atoms [3–5].

The trajectory of a classical ergodic system reaches all regions on the energy shell for sufficiently long times, establishing the microcanonical ensemble. As a consequence, suitable chosen subsystems obey the Boltzmann distribution. In the quantum case, switching on an interaction in a many-body system will combine the unperturbed eigenstates $|i\rangle$ of similar energies into new energy eigenstates: $|\alpha\rangle = \sum_i c_i^\alpha |i\rangle$. If the expectation values $A_\alpha = \langle\alpha|\hat{A}|\alpha\rangle$ of observables in these new eigenstates approach their microcanonical values $A_{\rm micro}(E)$, as obtained by averaging over all unperturbed states in a small energy window around E, then the properties of thermal equilibrium are established in each many-body eigenstate. This is the essential idea behind the 'eigenstate thermalization hypothesis' (ETH) [6, 7].

Recently, the ETH has been tested in numerical experiments [8–10], by means of exact diagonalization. For few-body observables like the momentum distribution, indeed it was demonstrated that $A_\alpha \approx A_{\rm micro}(E_\alpha)$ and that the fluctuations around $A_{\rm micro}$ decrease with increasing interaction strength and system size.

In the present work, we address the important question of how fast thermal equilibrium is approached when increasing the system size. A direct, brute-force numerical approach would be prohibitive. Instead, we characterize the gradual delocalization of eigenstates in the many-body Fock space via the inverse participation ratio (IPR) $\sum_{i=1}^{D}(p_i^\alpha)^2$ (with $p_i^\alpha = |c_i^\alpha|^2$) which turns out to be connected with the fluctuations of A_α. While a connection between the IPR and the fluctuations was

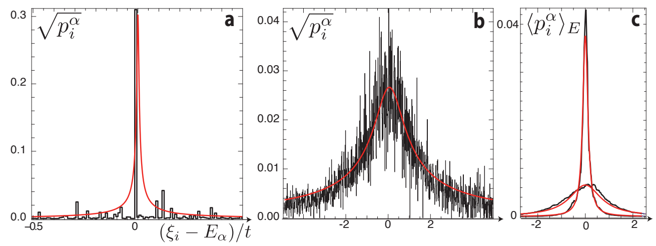

Figure 1. Probability distribution $p_i^\alpha = |\langle i|\alpha\rangle|^2$ of a many-body eigenstate $|\alpha\rangle$ in the non-interacting Fock basis (energies ξ_i). a) For weak interaction $V/t = 0.1$, the eigenstate is localized in Fock space, consisting of a few isolated peaks. b) At large $V/t = 1.3$, all Fock states with energies ξ_i close to E_α contribute. c) p_i^α averaged over a couple of nearby eigenstates in a range $\delta E/t = 0.05$, for $V/t = 0.45, 1.45$ (top, bottom). It can be approximated by a Lorentzian of width $\overline{\Gamma}$ (red line). The energy was chosen to correspond to infinite effective temperature (see main text).

observed recently [11, 12], we are able to conjecture its functional form and its dependence on system size and interaction strength, based on earlier analytical results on Fock-space localization by P. Silvestrov. In particular, we have numerical evidence that the interaction strength needed for thermalization is below that needed for full quantum chaos. Moreover, we find that in the thermodynamic limit (TDL) thermalization (in the sense of the ETH) sets in for arbitrarily small interactions. This is in contrast to recent observations on relaxation in a classical 1D system [13].

Here, we address these questions by means of exact numerical diagonalization for a system of spinless 1D fermions on a lattice, where integrability is broken by an interaction of strength V. As the observable of interest, we consider the fermionic momentum distribution $\hat{f}_k$. Our main result is that for large enough V the fluctuations of $f_k^\alpha \equiv \langle\alpha|\hat{f}_k|\alpha\rangle$ are determined by the IPR which roughly can be considered as the inverse number of non-interacting Fock states $|i\rangle$ contributing to $|\alpha\rangle$ (see e.g. [14]). The IPR itself keeps track of the transition from integrability to quantum chaos [11, 15] and it was conjec-

tured only recently that it might directly determine the deviations of steady state expectation values from the corresponding microcanonical value [16].
We observe *three different regimes*, depending on the interaction strength. An important scale is set by the mean level spacing Δ_f between Fock states that couple directly to a given initial Fock state. If the interaction is smaller than Δ_f, then the eigenstates are 'localized' in Fock space [17, 18] and experience only a perturbative correction due to the interaction (see Fig. 1a). For couplings beyond Δ_f, the eigenstates delocalize and remarkably the IPR decreases *exponentially* with V on a scale that depends on Δ_f. This scale essentially decreases polynomially in particle number and system size. Therefore, we expect the fluctuations of f_k^α to be suppressed to zero in the TDL even for vanishingly small interaction strength, establishing eigenstate thermalization of the considered observable. Increasing the interaction even further, eigenstates become chaotic (see Fig. 1b) and the IPR as well as the fluctuations in f_k^α decrease as the inverse many-body density of states as it was conjectured in [6, 7]. These results should apply rather generically to few-body observables diagonal in the eigenbasis of the unperturbed Hamiltonian.

Model. – We consider n spinless 1D fermions with periodic boundary conditions on a lattice of N sites and with a next-nearest neighbor interaction breaking the integrability of the system. The Hamiltonian reads:

$$\hat{H}_0 + \hat{V} = -t \sum_{i=1}^{N} \hat{c}_i^\dagger \hat{c}_{i+1} + \text{H.c.} \\ + V \sum_{i=1}^{N} (\hat{n}_i - 1/2)(\hat{n}_{i+2} - 1/2) \,. \qquad (1)$$

The eigenstates $|i\rangle$ of $\hat{H}_0$ with $\xi_i = \langle i|\hat{H}|i\rangle$ are given by the Fock states of n fermions in momentum space. Due to the translational symmetry, the interaction does not mix Fock states with different total momentum K. Therefore, each momentum sector K with dimension D_K will be considered separately.We exclude the $K = 0$-sector as it possesses a trivial extra symmetry under reflection. In our numerical examples $n = 7$ and $N = 21$.

Fluctuations and IPR. – In the following, we discuss the expectation values f_k^α of the momentum occupation numbers $\hat{f}_k = \hat{c}_k^\dagger \hat{c}_k$ (where $\hat{c}_k \equiv 1/\sqrt{N} \sum_{j=1}^{N} e^{-ikx_j} \hat{c}_j$). Being interested in the properties of typical eigenstates, we analyze the statistics of an ensemble of states $|\alpha\rangle$ with similar eigenenergies $E_\alpha \in I_E = [E - \delta E, E + \delta E]$, which will be called in the following 'eigenstate ensemble' (EE). The width of the energy window δE has to be chosen small enough to avoid artifacts resulting from systematic dependencies on E. Averages with respect to the EE are denoted by $\langle \ldots \rangle_E$. For not too large interactions, one can easily show that $\langle f_k^\alpha \rangle_E \approx f_{k,\text{micro}}(E)$. However, the crucial statement of the ETH is that for *each* eigenstate itself $f_k^\alpha \to f_{k,\text{micro}}$ when going to the TDL, i.e., that the

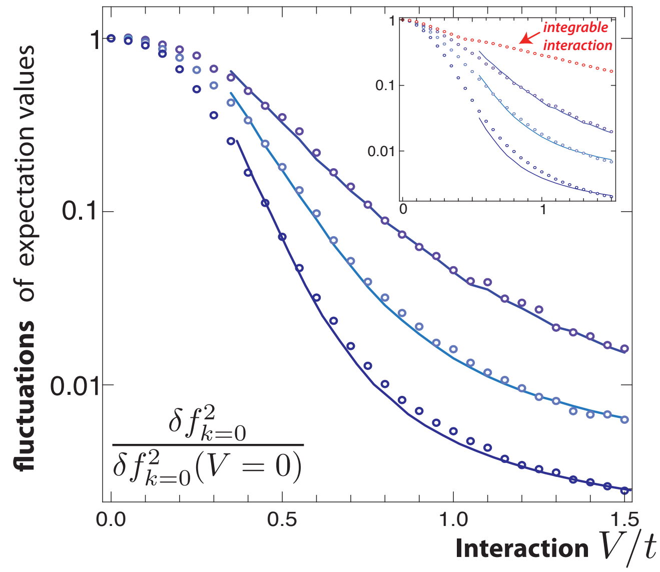

Figure 2. Fluctuations of expected occupation number $\langle\alpha|\hat{f}_k|\alpha\rangle$ between eigenstates decrease with increasing interaction strength V, indicating eigenstate thermalization. Plot shows the variance $\delta f_{k=0}^2$, for states with an effective temperature $T/t = 1.2, 1.7, \infty$ (from top to bottom), with energy shells of width $\delta E/t = 0.25$. Solid lines show const $\times \bar{f}_{k=0}(1 - \bar{f}_{k=0}) \sum_i \text{Var}_E(p_i^\alpha)$, with a slightly T-dependent constant. Finally, we averaged the results over all total momentum sectors K. Inset: As in main figure, but with δf_k^2 averaged over all k. The red dots show δf_k^2 averaged over all k for an integrable model with nearest-neighbor interactions (at $T = \infty$ and $K/(2\pi/N) = 1$). K-averages are only performed to improve statistics. The same results are obtained for individual K-sectors.

fluctuations of f_k^α from state to state vanish:

$$\delta f_k^2 \equiv \left\langle \left\{ f_k^\alpha - \overline{f_k} \right\}^2 \right\rangle_E \overset{N \to \infty}{\to} 0. \qquad (2)$$

We introduced the EE-variance δf_k^2 and $\overline{f_k} = \langle f_k^\alpha \rangle_E$. Representing f_k^α in the Fock basis $f_k^\alpha = \sum_{i=1}^{D_K} p_i^\alpha f_k^i$ (with $f_k^i = \langle i|\hat{f}_k|i\rangle$) this statement becomes plausible. For strong interaction, typical eigenstates are spread out widely in Fock space (Fig. 1b), i.e., they are composed of a large number of Fock states close in energy. Due to the law of large numbers, we thus expect the fluctuations to decay as the mean inverse number of Fock states contributing to $|\alpha\rangle$, i.e., as the mean IPR

$$\chi = \langle \sum_{i=1}^{D_K} (p_i^\alpha)^2 \rangle_E. \qquad (3)$$

Before deriving the connection between δf_k^2 and χ formally, we focus on the numerical results for the present model. Fig. 2 shows δf_k^2 as a function of V evaluated w.r.t. eigenstates at various energies. The eigenenergies can be re-expressed in terms of effective temperatures T, with $E_T \equiv \text{tr}_K(\hat{H} e^{-\hat{H}/T})/\text{tr}_K(e^{-\hat{H}/T})$. The results are compared to the IPR, or more precisely to

the sum over the variances $\mathrm{Var}_E(p_i^\alpha) = \langle (p_i^\alpha)^2 \rangle_E - \langle p_i^\alpha \rangle_E^2$ (see discussion below), clearly demonstrating that indeed $\delta f_k^2 \propto \sum_i \mathrm{Var}_E(p_i^\alpha)$ even for small interactions. This is in stark contrast to the case of integrability conserving nearest-neighbor interaction (inset Fig. 2), where the suppression of δf_k^2 with V is much smaller than in the prior case.

Formally, representing δf_k^2 in terms of p_i^α, one finds

$$\delta f_k^2 \simeq \overline{f}_k(1-\overline{f}_k) \sum_i \mathrm{Var}_E(p_i^\alpha) + \sum_{i \neq j}^{D_K} \delta f_k^{ij} \mathrm{Cov}_E(p_i^\alpha p_j^\alpha) \quad (4)$$

with $\delta f_k^{ij} = (f_k^i f_k^j - \overline{f}_k^2)$ and the covariance matrix $\mathrm{Cov}_E(p_i^\alpha p_j^\alpha) \equiv \langle p_i^\alpha p_j^\alpha \rangle_E - \langle p_i^\alpha \rangle_E \langle p_j^\alpha \rangle_E$. The first term in Eq. (4) contains the suppression of δf_k^2 with increasing number of Fock states contributing to a typical eigenstate. It is essentially determined by χ [we note $\chi \approx \sum_i \mathrm{Var}_E(p_i^\alpha)$ below the regime of full chaos (see below)]. We replaced $\sum_i (f_k^i - \overline{f}_k^2)\mathrm{Var}_E(p_i^\alpha) \to (\overline{f}_k - \overline{f}_k^2)\sum_i \mathrm{Var}_E(p_i^\alpha)$, which is justified as $\mathrm{Var}_E(p_i^\alpha)$ is a smooth function of i. The prefactor $\overline{f}_k(1-\overline{f}_k)$ is nothing but the variance of the momentum occupation numbers for the non-interacting case.

The off-diagonal contributions in Eq. (4) are sensitive to residual correlations within eigenstates and are expected to become small for strong perturbations. Surprisingly, for strong enough interactions, it approximately reproduces the diagonal part of Eq. (4). Thus, even though δf_k^2 is still determined by the IPR, one observes a deviation of the prefactor of $\mathcal{O}(1)$. A very similar observation was made in [19] while investigating finite fermionic systems with random two-body interactions and was traced back to the strong correlations between matrix elements of two-body interaction matrices.

To sum up, we find that the fluctuations in the expectation value of $\hat{f}_k$ from eigenstate to eigenstate are determined by the IPR χ. Thus, in the following, it will be discussed how χ decreases with increasing V and system size. Being a measure for the mean effective number of Fock states forming an eigenstate, χ indicates the 'delocalization' crossover in Fock space and serves as an indicator for the transition from integrability to quantum chaos.

Definitions – For the following discussion of the IPR, we need to set up a few technical definitions. We introduce the effective density $\rho_f^i(\omega)$ of Fock states $|j\rangle$ coupling to a state $|i\rangle$ of energy $\xi_i \in I_E$ (i.e., $\langle i|\hat{V}|j\rangle \neq 0$), where the energy difference between both states is $\xi_i - \xi_j = \omega$. Averaging over a couple of states $|i\rangle$ (indicated by $\langle \dots \rangle_E^0 = [\sum_{i,\xi_i \in I_E}]^{-1}[\sum_{i,\xi_i \in I_E} \dots])$ one obtains the *mean effective density of states* $\rho_f(\omega, E) = \langle \rho_f^i(\omega) \rangle_E^0$. Furthermore, it will be convenient to introduce the interaction formfactor

$$F(\omega, E) = \pi \langle \int_{\omega - \frac{\delta\omega}{2}}^{\omega + \frac{\delta\omega}{2}} \frac{d\omega'}{\delta\omega} \sum_{j=1; i \neq j}^{D_K} V_{ij}^2 \delta(\xi_j - \xi_i - \omega') \rangle_E^0 \quad (5)$$

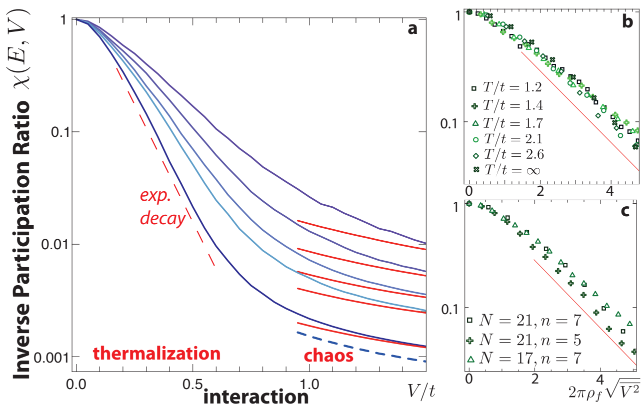

Figure 3. a) The inverse participation ratio χ decreases as many-body eigenstates get more delocalized for increasing interaction strength V. From top to bottom: Effective temperatures $T/t = 1.2, 1.4, 1.7, 2.6, \infty$ (blue lines; averaged over all momentum sectors). The most important feature is an exponential decay at intermediate interactions (dashed line; see Eq. (6)) followed by a power-law tail in the quantum chaotic regime, where it can be well approximated by Eq. (8) (shown only for $T = \infty$ and $K = 2\pi/N$: blue, dashed line). In the chaotic regime, the amplitudes c_i^α are Gaussian distributed, leading to $\chi \to 3\sum_i \langle p_i^\alpha \rangle_E^2$ (red lines). b) "Scaling plot": As before, but plotted vs. $2\pi\rho_f\sqrt{\overline{V^2}}$ (and only for a single K). c) Similar plot, but for various system sizes, at $T/t = \infty$.The red line displays Eq. (6), with $\mathcal{C} \approx 0.75$, for comparison.

This can be rewritten as $F = \pi\rho_f\overline{V^2}$, where $\overline{V^2}$ denotes a mean matrix element squared. For $\omega \to 0$ and small V, the form factor F reduces to Fermi's golden rule rate for a Fock state of energy E. In the following, only the mean matrix element and the effective density of states with respect to states close in energy, i.e., $\overline{V^2}(\omega \simeq 0, E)$ and $\rho_f(\omega \simeq 0, E)$ will appear. For brevity these will now be denoted by $\overline{V^2}$ and $\rho_f = \Delta_f^{-1}$, respectively.

Localized regime – As long as $\sqrt{\overline{V^2}} \ll \rho_f^{-1}$, eigenstates can be obtained within standard perturbation theory (apart from a small set of eigenstates, which can be traced back to degenerate Fock states). A given Fock state gets perturbed by the set of directly coupling states and eigenstates consist of a small number of sharp peaks (Fig. 1a), i.e., they are localized in Fock space.

Delocalization – Increasing the coupling strength $\sqrt{\overline{V^2}} \sim \rho_f^{-1}$, one enters the regime of *delocalized* eigenstates [18]. Perturbation theory breaks down and the IPR starts to decrease rapidly (see Fig. 3a). In this regime, the fluctuations δf_k^2 become directly determined by χ. Surprisingly, one observes an exponential decay of χ and we found good numerical evidence that

$$\chi \propto \exp\{-\mathcal{C}\rho_f\sqrt{\overline{V^2}}\}. \quad (6)$$

The numerical constant $\mathcal{C}$ is independent of temperature and system size. In Figs. 3b,c, the IPR is shown as a function of the scaling variable $2\pi\rho_f\sqrt{\overline{V^2}}$ for eigenstates

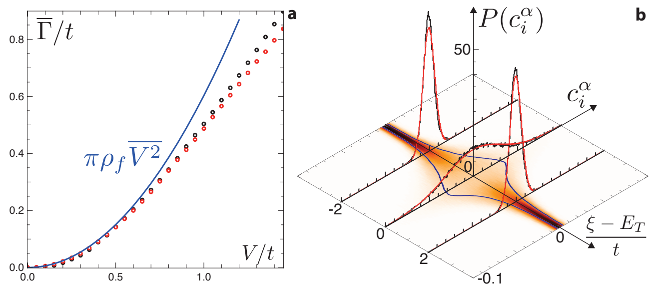

Figure 4. a) Fock state decay rate $\overline{\Gamma}$ vs. V (at $T = \infty$), extracted from the imaginary part of the self-energy (red dots). For small V, Fermi's golden rule $\overline{\Gamma} = \pi\rho_f\overline{V^2}$ holds, while $\overline{\Gamma}$ increases linearly in V for large V. For this plot, $\mathrm{Im}\Sigma_i(\omega)$ was averaged in both ω and energy ξ_i over the energy interval of width $\delta E = 0.25t$ centered around E_T. Black dots show the results of a direct fit of $\langle p_i^\alpha\rangle_E$. Here $K = 2\pi/N$. b) Amplitude distribution $P(c_i^\alpha)$ for eigenstates at $T/t = \infty$ with $\delta E/t = 0.25$ and $V/t = 1$ demonstrating that for very large V one enters the chaotic regime. In this regime, the amplitudes c_i^α are gaussian distributed as originally conjectured in [6]. In plane: energy dependent standard deviation $\pm[\langle(c_i^\alpha)^2\rangle_E]^{1/2}$ of P (blue lines). Out of plane: Cuts of P (black lines), which can be described by gaussians of variance $\langle(c_i^\alpha)^2\rangle_E$ (red lines).

at different energies E and for various N and n. Indeed, in good accordance to Eq. (6) all curves collapse to the same scaling curve. An explanation of this exponential decay of χ might be found in the two-particle nature of the interaction, following P. Silvestrov. In [20] it was argued (in a random matrix setting) that for moderate interaction strength, typical eigenstates are composed of independent pairs of interacting fermions. Thus, eigenstates decompose into direct products of pairs of Fock states, resulting in an exponential decay of χ, of the form given by Eq. (6). While this exponential decay (and additional corrections) have been confirmed numerically in a random quantum dot Hamiltonian [14], here we find it in a translationally invariant many-body system without disorder.

We now discuss the dependence on system size. The effective density of states $\rho_f(\omega)$ scales as N^3. For example, at large T, we have $\rho_f(\omega)t \simeq N^3\rho^2(1-\rho)^2 r(\omega)$, with the density ρ. For our particular model, $r(\omega) \propto \ln(t/\omega)$ for $\omega \to 0$ due to transitions of particle pairs around the inflection point of the $-2t\cos(k)$ dispersion, resulting in $\rho_f^{-1} \propto t/(N^3 \ln N)$ (assuming a cutoff scale $\omega/t \sim 1/N$). Together with the scaling of the matrix elements $\sqrt{\overline{V^2}}(\omega, E) = v(\omega, E)V/N$, this would yield $\chi \propto \exp\left\{-\tilde{C}N^2\ln N\rho^2(1-\rho)^2 V/t\right\}$, with $\tilde{C}$ being independent of N. Thus, we expect the fluctuations to decrease drastically in the thermodynamic limit even in this intermediate regime, where eigenstates are not yet ergodic.

Chaos – Only by increasing the interaction even further, one enters the regime of ergodic eigenstates. By 'ergodic eigenstates', we understand states which in principle are composed of all Fock states close in energy (cf. Fig. 1b). No Fock states are excluded a priori, e.g., due to the two-body nature of $\hat{V}$ or further symmetries from contributing to an ergodic eigenstate. The amplitudes c_i^α become Gaussian distributed random variables [6, 7] as it is shown in Fig. 4b with a Lorentzian variance [6, 21, 22]

$$\langle p_i^\alpha\rangle_E \simeq \frac{1}{\pi\rho_K(E)}\frac{\overline{\Gamma}(E-\xi_i, E)}{(\xi_i - E - \overline{\delta}(E,\xi_i))^2 + \overline{\Gamma}^2}, \qquad (7)$$

where ρ_K denotes the full many-body density of states for total momentum K, scaling as $(N-1)!/(N-n)!n!$. This indicates the crossover to full quantum chaos. We checked that in this regime the nearest neighbor level spacing statistics agrees with the GOE-Wigner surmise, characteristic for GOE random matrix ensembles. Due to the Gaussian distribution for c_i^α, one finds $\chi = 3\sum_\alpha\langle p_i^\alpha\rangle_E^2$ resulting in

$$\chi \simeq \frac{3}{2\pi}\frac{1}{\overline{\Gamma}(0,E)\rho_K(E)}, \qquad (8)$$

which is in fairly good agreement with the numerical results in Fig. (3a), demonstrating the suppression of δf_k^2 by the inverse many-body density of states as it was conjectured in [6, 7]. The mean spreading width $\overline{\Gamma}$ (Fig. 4a) can be extracted from the Fock state self-energy Σ by averaging $-\mathrm{Im}\Sigma(\xi_i, \omega)$ over $\xi_i, \omega \in I_E$. Σ is obtained from $G(\xi_i, \omega) \equiv \langle i|[\omega + i0^+ - \hat{H}]^{-1}|i\rangle$ via $G \equiv [\omega + i0^+ - \xi_i - \Sigma]^{-1}$. Fig. 1c shows a comparison of $\langle p_i^\alpha\rangle_E$ and a Lorentzian of width $\overline{\Gamma}$ extracted directly from $-\mathrm{Im}\Sigma$.

The important question remains, how the second crossover scale (governing the crossover from delocalized to ergodic eigenstates) depends on system size. We found some indication that it might depend on the intensive 'energy range' W of the coupling matrix $\hat{V}$. Consider the dependence of $\overline{\Gamma}$ on V in Fig. 4a. For small V, Fermi's golden rule applies and one finds $\overline{\Gamma}(0,E) \simeq F(0,E) \propto V^2/t$. For large V, one observes a crossover $\overline{\Gamma} \propto V^2/t \to \overline{\Gamma} \propto V$ indicating the entrance into the strong coupling regime, where $\overline{\Gamma}$ and the finite width (in ω) of the formfactor F become comparable [21]. Comparing Figs. 3a and 4a, there might exist a close relation between this crossover and the onset of ergodicity of eigenstates. This would imply that the interaction energy scale ρ_f^{-1} for the onset of thermalization is parametrically smaller than the scale for the transition to chaos, determined by W.

Conclusions. – By means of exact diagonalization we investigated the interaction induced onset of eigenstate thermalization in a system of 1D fermions. We found that the fluctuations of the expectation value of the momentum occupation number from state to state are proportional to the inverse participation ratio of eigenstates. For small interactions the latter decays exponentially before one enters the chaotic regime. The interaction scale for the onset of this decay is essentially set by the effective mean level spacing between interacting Fock states,

and this vanishes in the TDL. Thus, we corroborate the physical expectation that in the TDL at arbitrarily small interactions, eigenstate thermalization sets in.

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